Vibrational spectroscopy under an accessible computational microscope

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In the last 10 years, the concurrent progress in theoretical methods, computational power, and informatics, had a transformative impact on the prediction of vibrational spectra using the basic laws of quantum mechanics, which has been for a long time the domain of highly specialized computational scientists. I will discuss our conceptual and practical developments, beginning with the achievement of advanced and efficient treatment of the chemistry of localized electrons – the self-consistent DFT+U+V method. By this approach, I demonstrate remarkable agreement with experimental Raman spectra of complex Li-ions cathodes and other transition-metal compounds. I will then introduce our effort to automatizing and making accessible, through user-friendly workflows and a web-based GUI, the calculation of vibrational spectra (infrared, Raman, INS) for realistic applications. The entire framework is openly available, facilitating the cooperation among researchers of different communities and leading the wide-spread use of advanced simulation capabilities.